
Pre-melting phenomena in an fcc metal

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Abstract

The Earth's core is believed to be made of an iron-nickel alloy with a few percent of light elements, but its precise structure and composition still remain unknown. Seismological models in the Earth's inner core do not agree with mineralogical models resulting from *ab initio* calculations which predict shear-wave velocities up to 30% greater than seismically observed values. Recent computer calculations revealed that this difference may be explained by a dramatic, non-linear, softening of the elastic constants of Fe just before melting, interpreted as "pre-melting" effects.

To date, computer simulations are the only result on pre-melting of direct applicability to the Earth's core and it is crucial to investigate such phenomena at inner core conditions. Measuring the pressure dependence of pre-melting effects at such extreme pressures and temperatures to the required precision is, however, exceedingly challenging.

We investigated to what extent pre-melting behaviour occurs in the physical properties of other metals at more experimentally tractable conditions. In particular, we determined the thermal expansion of gold (Au) by X-ray powder diffraction from 40 K up to the melting point (1337 K). Au is an ideal test material as it crystallises in a simple monatomic face-centred cubic structure and has a relatively low melting temperature making it a candidate material to study in the laboratory.

Over the temperature range investigated the behaviour of the material may be adequately described by a Grüneisen approximation to the zero-pressure equation of state representing the thermal expansion of the "perfect crystal", combined with the theory of thermodynamics of point defects to include the contributions from lattice defects at high temperature ("real crystal"). Au shows a non-linear increase in thermal expansion prior to melting, which is likely due to the generation of point defects over a large range of temperature, beginning at $T/T_m > 0.75$, which is very similar to what has been observed in the elastic moduli.

From the present study it appears that pre-melting phenomena in *fcc* metals may be less pronounced than those observed in *hcp* metals, such as Fe, at Earth's inner core conditions.

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